periplanone-B

Inchi: InChI=1S/C15H20O3/c1-9(2)11-5-4-10(3)6-12-14(18-12)15(8-17-15)13(16)7-11/h4-5,9,1
InchiKey: KVFSFBCTIZBPRK-UFURTSHJSA-N
Formula: C15H20O3
SMILES: C=C1C=CC(C(C)C)CC(=O)C2(CO2)C2OC2C1
Mol. weight [g/mol]: 248.32

Physical Properties

Property code	Value	Unit	Source
gf	-18.16	kJ/mol	Joback Method
hf	-429.23	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	61.28	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.270		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
ripol	2619.00		NIST Webbook
tb	695.07	K	Joback Method
tc	939.26	K	Joback Method
tf	439.01	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.52	J/mol×K	695.07	Joback Method
cpg	614.33	J/mol×K	735.77	Joback Method
cpg	633.96	J/mol×K	776.47	Joback Method
cpg	652.59	J/mol×K	817.16	Joback Method
cpg	670.42	J/mol×K	857.86	Joback Method
cpg	687.62	J/mol×K	898.56	Joback Method
cpg	704.39	J/mol×K	939.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R494812&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume